

Diisopropyl fluorophosphate
55-91-4 | DTXSID1040667

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.23e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 6.30e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diisopropyl fluorophosphate</div> <div>Measured: 8.36e-02</div> <div>Predicted: 8.23e-02</div>	<div>Image not found</div> <div>Pinacolyl methylphosphonofluoridate</div> <div>Measured: 1.15e-01</div> <div>Predicted: 1.33e-01</div>	<div>Image not found</div> <div>Ethyl 4,4,4-trifluoroacetoacetate</div> <div>Measured: 4.35e-02</div> <div>Predicted: 7.99e-02</div>
<div>Image not found</div> <div>Cyclosarin</div> <div>Measured: 2.05e-02</div> <div>Predicted: 5.91e-02</div>	<div>Image not found</div> <div>Mipafox</div> <div>Measured: 4.39e-01</div> <div>Predicted: 4.12e-01</div>	